Focalization : A numerical test for smoothing effects of collision operators

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S. Cordier*, B.Lucquin-Desreux† and S. Mancini†

Abstract

This paper deals with the numerical analysis of the focalization of a beam of particles. In particular, this model can be useful to check whether or not the cut-off Boltzmann equation leads to some kind of smoothing effect as for the Fokker-Planck-Landau equation.

Key Words: Kinetic model, focalization of a beam, collision operator (Boltzmann, Fokker-Planck, Lorentz), smoothing effects, propagation of singularity

1 INTRODUCTION

In this paper, we are interested in the evolution of a system of particles injected in a bounded region all with the same velocity and undergoing collisions with heavier particles present in the domain. When a particle (e.g. a photon) collides with a heavier particle (e.g. neutron or ions) we can consider that the collision is elastic: the velocity modulus does not vary (or equivalently, the kinetic energy is conserved); the velocity modulus can be treated as a parameter of the problem. On the other hand, the velocity direction is changed by the scattering event. This behavior is modeled by the so called Boltzmann-Lorentz collision operator (see [6]), which in the two-dimensional case reads:

$$Q_{BL}f(\theta) = \int_{S^1} B(\theta-\theta')\,(f(\theta')-f(\theta))\,d\theta'. \tag{1.1}$$

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When collisions become grazing, (see [5, 7, 10]) the Boltzmann-Lorentz operator converges to the Fokker-Planck-Lorentz (or Laplace-Beltrami) operator (see [2, 11]):

$$Q_{FP}f(\theta) = \partial^2_{\theta\theta} f. \tag{1.2}$$

The focalization of a beam of particles is a test used in photonics. It consists in studying the evolution of a beam of photons injected in a bounded region from one side of the boundary with velocity close to the speed of light and perpendicular to the boundary. Inside the region, the photons may collide with neutrons or ions and change their trajectory, or may freely move from one side to the other one a straight line without changing their velocity direction. In this paper, we investigate the rate of particles reaching the opposite side of the domain (in the one-dimensional space case a slab) with a velocity direction equal to the incoming one (in a slab, perpendicular to the planes). It seems clear that the number of particles reaching the opposite side of the domain depends on the amount of collisions that they undergo. We call $\mathcal{F}$ the *focalization* coefficient, i.e. the rate of particles which exit the domain with the same velocity direction they had when entering the region (i.e. in the slab with a perpendicular velocity direction). We will show how this simple model may be useful to check whether or not the cut-off Boltzmann equation leads to some kind of smoothing effect as the Fokker-Planck-Landau equation.

This paper is organized as follows. In section 2 we introduce the transport equation modeling the evolution of a beam of particles. This model is one-dimensional in space and two-dimensional in velocity. In section 3 we discuss the smoothing effect of the collision operators (Boltzmann-Lorentz and Fokker-Planck-Lorentz) on singular data. In section 4 we present the numerical result validating our analysis. Finally, in section 5, we summarize our results and discuss those that would be obtained by other numerical approximations.

2 THE MODEL

Let us consider a system of particles with velocities v of modulus $|v| = 1$ and which undergo elastic collisions. The evolution of this system of particles is described by the distribution function $f = f(x, \theta, t)$ representing the number of particles which, at time $t > 0$, are in a position $x \in [0, 1]$, with velocity $v = (\cos\theta, \sin\theta)$, $\theta \in \mathbb{R}/2\pi\mathbb{Z}$. The distribution function satisfies an equation of the form:

$$\partial_t f + \cos\theta\,\partial_x f = \frac{1}{\tau} Q(f), \tag{2.3}$$

where τ is the collision relaxation time, and Q is either the isotropic Boltzmann-Lorentz operator:

$$Q_{BL}(f)(\theta) = < f > - f \ , \quad < f > = \frac{1}{2\pi} \int_0^{2\pi} f(x, \theta, t) \, d\theta, \tag{2.4}$$

or the Fokker-Planck-Lorentz (or Laplace-Beltrami) operator (1.2).

Note that this problem is one-dimensional in x and two-dimensional in v. The length of the domain where the evolution of the system of particles occurs is rescaled to one (this is related to a change of collision time as explained in [4]).

We complete equation (2.3) with the initial data $f(t = 0) = 0$ and the following incoming boundary conditions:

$$\begin{aligned} f(x = 0, \theta, t) &= g(\theta, t) \ , \quad \text{for } \theta \in [-\pi/2, \pi/2] \\ f(x = 1, \theta, t) &= 0 \ , \quad \text{for } \theta \in [\pi/2, 3\pi/2]. \end{aligned} \tag{2.5}$$

These boundary conditions model an entering beam of particles on the left hand side ($x = 0$) of the slab and no re-entering particle flux on the right hand side ($x = 1$). We assume that the beam is well focalized with a velocity perpendicular to the region where collisions occur, the entering profile g can be considered as a Dirac mass along the direction $\theta = 0$

$$g(\theta, t) = \delta_{\theta=0}, \forall t > 0. \tag{2.6}$$

We note that if there were no collision (i.e. $\tau \to \infty$), every particle would be transmitted, i.e. it would cross the domain in a time $T = 1$ and exit with the same velocity direction $\theta = 0$. In other words, all the particles in absence of collisions would travel along a straight line and their velocity would not vary (nor in modulus nor in direction).

On the other hand, if there are many collisions in the region (i.e. $\tau \to 0$), then the particles of the beam entering the domain are reflected, i.e. they exit the domain on the same side, $x = 0$. Moreover, a very small number of particles will reach the opposite boundary of the domain, i.e. $x = 1$, and an even smaller number of them will have the velocity direction $\theta = 0$. In other words, the beam is mostly reflected and the number of particles reaching the opposite side of the domain with the right velocity direction is negligible.

Finally, for $0 < \tau < \infty$, e.g. $\tau = \mathcal{O}(1)$, some of the particles are transmitted, others are reflected. We say that a stationary solution is reached when the flux of outgoing particles (either transmitted or reflected) equals the flux of incoming particles.

Recently, this focalization problem has been studied in the 3-dimensional [4] and 2-dimensional [12] contexts. In both cases, the curve of the focalization coefficient is given as a function of the relaxation time τ and mainly concerns the case of the Fokker-Planck operator.

The dependence of the solution on singular data has been studied in the space homogeneous case, see for instance [7, 14]. Concerning the space inhomogeneous case, propagation of singularities has been proven under the cut-off assumption in [1]; one can also find some regularity results for the non cut-off case for a particular Boltzmann type operator in [8].

The aim of this paper is to try to characterize at a numerical level, by use of an efficient and simple test case, these regularizing (or non regularizing) properties.

3 SMOOTHING EFFECTS

We expect the solution to keep in time its singularity in the Boltzmann case. On the contrary, in the Fokker-Planck case, the solution is instantaneously regularized. As a matter of fact, let us first consider the space-homogeneous problem $\partial_t f = Qf$, with $f = f(\theta, t)$ independent on x, and initial data given by:

$$f(\theta, 0) = \delta_{\theta=0}$$

(by analogy with the boundary conditions (2.5),(2.6) at time $t = 0$). The solution in the Boltzmann-Lorentz case (i.e. $Q = Q_{BL}$ with $\tau = 1$) is given by:

$$f(\theta, t) = \delta_{\theta=0} \exp(-t) + (1 - \exp(-t))1/2\pi, \tag{3.7}$$

where we have used the fact that $\partial_t < f >= 0$, so that $< f >= 1$. It is easy to see that this solution converges towards a constant equilibrium state, but a singular, measured value part remains for any finite time (with an exponential decay with respect to time).

In the Laplace-Beltrami case (i.e. $Q = Q_{FP}$ with $\tau = 1$), the solution of the space-homogeneous problem is the elementary solution of the heat equation with periodic conditions:

$$f(\theta, t) = \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} \exp(-n^2 t) \exp(in\theta), \quad t > 0.$$

In this case, the singularity of the Dirac at initial time disappears for any $t > 0$ and the solution is smooth with respect to θ, as seen on the exponential decay of the Fourier coefficients.

On the other hand, it has been proven that the Fokker-Planck-Landau operator regularizes the solution as it is done for the heat equation (see [14]). In the non homogeneous case, the singularities are propagated along the characteristics in the cut-off Boltzmann case, i.e. when the cross section is integrable and the lost and gain terms can be separated (see [1]); whereas, in the non cut-off case, some smoothing effect occurs for a particular Boltzmann type operator (see [8]).

Concerning problem (2.3), although no analytical solution in the non-homogeneous case is known, it is believed that the solution will have the same properties than in the space-homogeneous case: the singularity will follow the characteristics in the Boltzmann-Lorentz case, whereas the solution will instantaneously become smooth in the Laplace-Beltrami case.

4 NUMERICAL METHOD AND RESULTS

From now on we assume that the relaxation time is $\tau = 1$. Let us approximate the distribution function on a uniform grid both in space $x = x_i = i\Delta x$, $\Delta x = 1/N_x$ and $i = 0...Nx$, and in velocity angle $\theta = \theta_j = -\pi + j\Delta\theta$, $\Delta\theta = 2\pi/N_\theta$ and $j = 0...N_\theta - 1$. The scheme is based on a time splitting:

- one time step for the transport equation using an explicit upwind scheme with time step restriction for preserving stability (and positiveness): $\Delta t = \Delta x$ (we choose a CFL condition equal to 1 to avoid numerical dissipation)

- one time step for the collision part which is solved using either a classical second order quadrature formula in the Boltzmann case, or a second order finite difference scheme in the Fokker-Planck case. Note that one can also use the exact solution known for the Boltzmann case (see equation (3.7)). Moreover, this part is treated implicitly so that there is no time step condition on this part. We also refer to [4] and [12] for an implicit finite element approximation respectively in 2D and 3D (with respect to the velocity variable).

The time needed for the first particle entering the domain to exit (if no collision occurs) is $T = L/|v| = 1$. We remark that the solution reaches its stationary equilibrium for $T = 10$ (200 iterations). The number of time iterations to reach a given time is proportional to the number of points in the space discretization. We choose $N_x = 20$ and we are interested with the limit $N_\theta \to \infty$.

In Figure 1, we plot the outgoing distribution function against velocity. The initial Dirac mass is instantaneously smoothed by means of the Fokker-Planck operator, whereas in the case of the Boltzmann operator the distribution function is still picked.

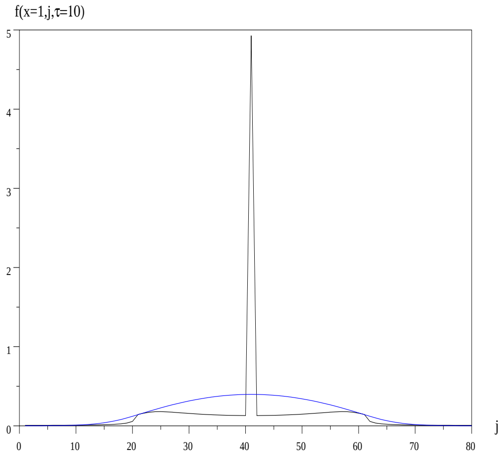

Figure 1: *The outgoing profile* $f(x = 1, \cdot, T = 10)$ *versus the index* j *of the velocity angle* θ_j *in the Boltzmann and Fokker-Planck case* $(N_\theta = 80)$

In order to differentiate the two cases (Boltzmann and Fokker-Planck), we refine the mesh with respect to θ. When doing this, we expect the focalization coefficient either to converge to 0 (in the Fokker-Planck case), or to a non-vanishing limit value (in the Boltzmann case). This is exactly what we observe in Figure 2, where we plot the focalization coefficient in terms of the number of iterations and for different numbers N_θ of discretization points in θ. We observe that in the Boltzmann case (on the left) this coefficient tends to a finite non zero value when $N_\theta \to \infty$ ($\theta = 0$ being a grid point there are still particles in this direction even when refining the grid). Whereas it rapidly goes to zero in the Fokker-Planck case (on the right). This is due to the fact that, the beam diffusing on more and more neighboring grid points, the number of particles which velocity precisely remains in the direction $\theta = 0$ decreases more and more and finally vanishes.

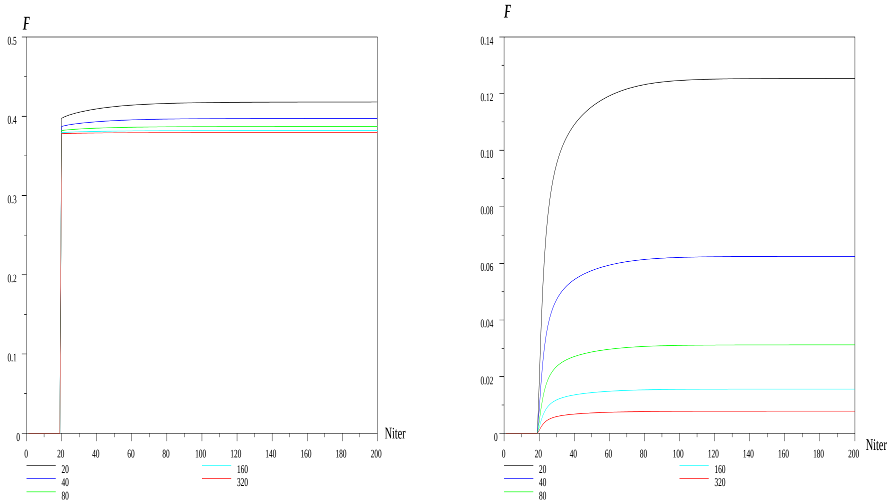

Figure 2: *The focalization coefficient against the number of iterations in the Boltzmann-Lorentz case (left), and in the Fokker-Planck-Lorentz case (right)*

In Figure 3, we also consider the case of Coulomb type operators, i.e. with a truncation around the value $\theta = 0$. More precisely, we consider operators of the form (1.1), where the kernel B now depends on a small truncation parameter ε in the following way (χ denotes the characteristic function):

$$B(z) = B^{\varepsilon}(z) = C_{\alpha,\varepsilon}\chi_{\{|z|>\varepsilon\}}|z|^{-\alpha},$$

for some α, $\alpha \geq 0$, where the constant $C_{\alpha,\varepsilon}$ is given by: $C_{\alpha,\varepsilon} = 1$ for $\alpha \in [0,3[$, $C_{\alpha,\varepsilon} = 1/\log\varepsilon$ for $\alpha = 3$ and $C_{\alpha,\varepsilon} = 1/\varepsilon^{3-\alpha}$ for $\alpha > 3$.

When ε goes to zero, the kernel of the Boltzmann-Lorentz operator has an integrable singularity for $\alpha < 1$, which allows to separate in the integral the gain term and the loss term: this corresponds to the so-called Grad's assumption of "angular cut-off". On the other hand, for $\alpha \geq 1$, there is a non integrable singularity around $\theta = 0$, but a Taylor expansion in the integral shows that there is a compensation between the gain and loss term (see [2] and [5]): these values of the parameter α correspond to the "non cut-off" assumption. Moreover, for $\alpha \geq 3$, the Boltzmann-Lorentz operator Q^{ε}_{BL} associated with this kernel B^{ε} converges (up to a fixed multiplicative constant) to Q_{FP} when ε goes to zero (see [2]); the case $\alpha = 3$ exactly corresponds to the Coulomb case.

We expect the focalization test to give the same results for the cut-off assumption (for example with $\alpha = 0.95 < 1$) than in the (isotropic)

Boltzmann case, i.e. that the focalization coefficient, which is precisely defined by:

$$\mathcal{F}(t) = \frac{f(x=1, \theta=0, t)}{f(x=0, \theta=0, t)}$$

converges to a fixed non zero value, when refining the grid with respect to the angle. On the contrary, we expect that this coefficient will go to zero in the "non cut-off" case (for example for $\alpha = 2$ or $\alpha = 3$), where an instantaneous regularization of the beam will occur, as for the Fokker-Plank-Lorentz case. These facts have been effectively confirmed by our numerical simulations, has shown in Figure 3, where in the last column we have quoted the ratio $\mathcal{R}$ between the focalization coefficient for $N_\theta = 320$, $\mathcal{F}_{320}$, and the same coefficient for $N_\theta = 160$, $\mathcal{F}_{160}$.

$\mathcal{F}$ for	$N_\theta = 320$	$N_\theta = 160$	$\mathcal{R} = \mathcal{F}_{320}/\mathcal{F}_{160}$
Boltzmann-Lorentz	0.3794	0.3819	0.9934
$\alpha = 0.95$	0.2137	0.2066	1.0344
$\alpha = 1$	0.1584	0.1624	0.9753
$\alpha = 1.1$	0.0771	0.0939	0.8211
$\alpha = 2$	0.0066	0.0133	0.4962
$\alpha = 3$	0.0036	0.0078	0.4615
Laplace-Beltrami	0.0078	0.0156	0.5

Figure 3: *Focalization coefficient,* $N_{iter} = 200$

We note that in the limit case $\alpha = 1$ the focalization coefficient behaves like in the Boltzmann-Lorentz case; this is not quite surprising, since this corresponds to the limit case where the compensation between the gain and loss terms is the weaker one. We also remark a very sharp decrease of the ratio $\mathcal{R}$ around the "critical" value $\alpha = 1$.

Let us finally remark that this focalization coefficient also naturally depends on the space (and time, since $\Delta t = \Delta x$) discretization. For example, by changing N_x from 10 to 20, one obtains a result for $N_\theta = 320$ which differs from 2.24% in the isotropic (Boltzmann-Lorentz) case. But we also observe that the relative variation of the ratio $\mathcal{R}$, which is in fact the "right" coefficient which allows to distinguish the regularizing case (i.e. the non cut-off case) from the Boltzmann one, is only of 0.04%. Also the relative error decreases when refining the mesh with respect to space (and time): by changing N_x from 20 to 40, the relative error on the focalization coefficient with $N_\theta = 320$ is of 1.18% and on the ratio $\mathcal{R}$ it is of order 0.03%. These errors are a bit more important in the Coulomb case ($\alpha = 3$): between the case $N_x = 20$ and $N_x = 40$, they are of the order 5.5% for the focalization coefficient with $N_\theta = 320$, and of order 3.08% for the ratio $\mathcal{R}$, which is still quite reasonable.

5 CONCLUSION

Note that the smoothing effect can also be observed using other methods: Monte Carlo or spectral methods.

- Using stochastic or Monte Carlo methods, the distribution function is represented by pseudo-particles. The numerical method is based on a time splitting: one time step solving the transport part, one time step for collisions.

  In the Boltzmann case (see [3, 9]), the method consists in performing a change of the particles velocity (choosing a post-collision velocity uniformly on the sphere) according to a random variable related to the collision time. It can be checked that the probability P of a particle exiting the domain without changing its velocity is not vanishing; more precisely, $P = \exp(-L/\tau)$, where L is the length of the domain, and τ is the collision time.

  In the Fokker-Planck (or Laplace-Beltrami) case, the solution can be obtained either using the grazing collision limit, by making a large number of small deviations, or using that for small time steps. The solution of the collision part for a Dirac initial data behaves as a Gaussian with variance related to the time step. Thus, the velocities are chosen according to a Gaussian distribution. Moreover, the probability P of exiting the domain with the velocity of the beam is zero. This property can be used to separate the case of Boltzmann operator ($P \neq 0$) and of Fokker-Planck operator ($P = 0$).

- The same holds true in the spectral method (see [13]). First, let us recall that the smoothness of a function is related to the decay of its Fourier coefficients (e.g. the Dirac measure corresponds to constant Fourier coefficients). When using a spectral method, the distribution function in velocity (or equivalently in angle) is represented by its Fourier coefficients. In the case of the Boltzmann operator, the distribution function at the right hand side has a singularity and thus the Fourier coefficients a_k at $x = L$ have a non zero limit when k goes to ∞. Concerning the Fokker-Planck (or Laplace-Beltrami) operator, the Fourier coefficients go to 0 as $k \to \infty$ (exponentially fast). The difficulty with spectral methods is that the representation of Dirac masses requires a large number of modes.

The same differentiation should be observed on the classical non linear Boltzmann operator (for binary collision) - in which case the singularities follow the characteristics, see [1] - and Fokker-Planck-Landau or non cutoff Boltzmann equation - in which case, regularity occurs, see [14] and [8]. Thus, this test serves to check smoothing effects, whatever the method is used for numerical simulations (discrete velocity, spectral or Monte Carlo methods).

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